

Critical properties of a continuous family of XY noncollinear magnets

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Monte Carlo methods are used to study a family of three dimensional XY frustrated models interpolating continuously between the stacked triangular antiferromagnets and a variant of this model for which a local rigidity constraint is imposed. Our study leads us to conclude that generically weak first order behavior occurs in this family of models in agreement with a recent nonperturbative renormalization group description of frustrated magnets.

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In spite of intensive study during the last 25 years the critical behavior of XY or Heisenberg frustrated magnets with a noncollinear ground state is still a strongly debated topic (see Refs. [1, 2] and references therein). This is, for instance, the case of the celebrated XY Stacked Triangular Antiferromagnet (STA) that we consider here, whose Hamiltonian is:

$$H = - \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad (1)$$

where the \mathbf{S}_i are two-component vectors and the sum runs over all pairs of nearest neighbor spins on a stacked triangular lattice. In Eq. (1), the in-plane interactions are antiferromagnetic ($J < 0$) and the inter-plane interactions are taken to be ferromagnetic ($J > 0$) with $|J| = 1$. The competition between the in-plane antiferromagnetic interactions produces a ground state where the three spins \mathbf{S}_1 , \mathbf{S}_2 and \mathbf{S}_3 on each elementary triangular plaquette are oriented at 120° one to another, that is:

$$\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 = \mathbf{0}. \quad (2)$$

For such a system, the order parameter is given by two orthogonal vectors of the same norm, a fact that has led to the hypothesis that noncollinear magnets could undergo a second order phase transition associated with a new — chiral — universality class [3].

However, it is now becoming more and more widely accepted that the physics of frustrated magnets is not given by such a simple picture [1, 4, 5, 6]. The complexity of the critical behavior of STA systems is exemplified in the experimental results (for a review see Ref. [1] and references therein). Indeed, scaling behavior is generally

found while universality is violated since materials which belong, *a priori*, to the same universality class display different critical exponents. It is thus difficult to interpret the experimental data within the usual picture of critical phenomena.

On the theoretical side, the situation is controversial [1, 5]. A nonperturbative renormalization group (NPRG) method [1, 4] finds that the phase transitions in these systems are *generically* weakly first order with the possibility of standard strongly first order transitions. More precisely while there is no RG fixed point there exists a whole region where the RG flow is very slow, corresponding to large — but finite — correlation lengths at the transition, which allows one to compute pseudo-critical exponents. Hence the violation of universality observed experimentally has a natural explanation since, in the absence of a fixed point, the pseudo-critical exponents found depend on the microscopic Hamiltonians. On the other hand, Pelissetto *et al.* have derived and resummed the six-loop β functions in three dimensions [7]. They find a fixed point and therefore predict a second order phase transition. Calabrese *et al.* have claimed that the lack of universality found can be accounted for by the spiral nature of the approach to the *focus* fixed point [5].

Our aim is to discriminate by means of numerical simulations between these two scenarios that both predict scaling behavior with varying critical exponents but differ in the predicted asymptotic behavior for temperatures very close to the transition temperature. Different systems having the same symmetry breaking scheme as XY-STA but differing by microscopic details have been

studied numerically [8, 9, 10, 11, 12, 13, 14, 15]. Apart from STA, they have *all* been found to undergo first order transitions [8, 9, 10, 11]. As for STA itself early numerical simulations favor a continuous transition [12, 13, 14, 15]. However the most recent simulation performed with lattice sizes much larger than those considered previously leads to first order behavior [11]. Thus, although there are now strong indications in favor of the nonperturbative scenario, the numerical evidence is still too weak to lead to a definite conclusion. In order to shed some light on this problem we consider a family of models, built up as generalizations of STA. We find that they *all* exhibit either strong first order transitions or a scaling behavior with varying exponents associated with a weak first order phase transition.

To perform our study we partition the original triangular lattice — with lattice spacing a — into elementary plaquettes labelled by an index I . They are composed of three spins $\mathbf{S}_1^I, \mathbf{S}_2^I$ and \mathbf{S}_3^I . The super lattice made of these plaquettes is, again, a triangular lattice, with lattice spacing $\sqrt{3}a$. The family of models we consider is defined by:

$$H(r) = - \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + r \sum_I (\mathbf{S}_1^I + \mathbf{S}_2^I + \mathbf{S}_3^I)^2 \quad (3)$$

where the first term is the same as in Eq. (1) and where the sum over I in the second r -term runs over the indices of the super lattice. For $r < -0.5|J|$, the ground state has the spins aligned ferromagnetically within a plaquette but are oriented at 120° from plaquette to plaquette; this is not the ground state expected for real materials. For $r = -0.5|J|$ the interactions inside the plaquettes vanish and the lattice becomes effectively a stacked Kagome lattice. For $r > -0.5|J|$ the ground state and thus the symmetry breaking scheme and order parameter are identical to those of the STA model, Eq.(1); we thus focus on this range of values in the following. For any value of $r > 0$ the r -term favors locally, that is *inside* the plaquettes, the 120° ground state configuration. It thus penalizes the relative fluctuations of the spins $\mathbf{S}_1^I, \mathbf{S}_2^I$ and \mathbf{S}_3^I inside a plaquette but still lets the orientation of the three-spin structure freely fluctuate from plaquette to plaquette. Note that, since the fluctuations of the spins inside a plaquette are noncritical, the r -term should not alter the critical physics of the STA *if* it is universal — see below. The $r \rightarrow \infty$ limit consists of a STA for which the ground state 120° structure is locally imposed at *all* temperatures. This model is called the STAR (R for rigid). Continuous changes in the ‘rigidity parameter’ r from zero to infinity thus correspond to a continuous change from the STA to the STAR. The STAR has been studied by Loison and Schotte [10] and has been found to undergo a strong first order transition. This already shows that, in fact, the critical behaviors of STA-like systems strongly depend on the microscopic details of the model.

r	T^*	β	γ	ν	η
0.0	1.458(2)	0.253(10)	1.13(5)	0.54(2)	-
0.2	1.5494(4)	0.249(6)	1.1(1)	0.531(20)	-0.06(2)
0.5	1.6420(3)	0.243(9)	1.04(10)	0.518(20)	-0.08(4)
0.8	1.7039(7)	0.218(10)	1.0(1)	0.490(20)	-0.04(3)
1.0	1.737(1)	0.213(9)	1.0(2)	0.482(25)	-0.07(3)

TABLE I: Critical exponents for various r . The results for $r = 0$ were obtained in [13].

We use a classical Monte Carlo Metropolis algorithm [16] to study this generalized model as a function of temperature and the rigidity parameter r . A number of different thermodynamic quantities have been computed with $0 \leq r \leq 8$ for lattices of linear sizes $L = 18$ to $L = 138$. In order to reduce the critical slowing down at the transition, each simulation run starts from a disordered state at a temperature well above the transition temperature and is slowly cooled to low temperatures. The system is allowed to equilibrate for 3×10^5 Monte Carlo sweeps (MCS) and the averages were performed over 5.5×10^5 steps. In order to avoid correlations between subsequent measurements, 20 – 30 Monte Carlo sweeps were performed between measurements.

$0 \leq r \leq 1.0$: *the weak first order region.* We begin our discussion with the small r region which is the most interesting one since real compounds are supposed to be close to STA. Moreover, for some of these compounds as well as for STA with $r = 0$ scaling behavior is found [1]. Since scaling laws are found to hold in this range of r , we analyze them by means of the standard methodology used for second order phase transitions. The fourth order cumulant U_M of the order parameter displays behavior characteristic of a second order transition and can be used to estimate the transition temperature T^* . We have determined T^* , the order parameter critical exponent β , the correlation length exponent ν , the susceptibility exponent γ and the anomalous dimension exponent η using finite size scaling (FSS) methods [13]. For appropriate values of T^* and of β and ν , the data should collapse onto a single curve. A sample log-log finite size scaling plot of the order parameter M for $r = 1.0$ is shown in figure 1. A similar FSS analysis of the susceptibility also satisfies scaling and can be used to determine γ . For sizes $L = 48, 60$ there are some deviations from scaling at small values of the reduced temperature t .

At T^* , the structure factor depends on system size as $S(\vec{Q}, L) \sim L^{2-\eta}$ where the exponent η is the anomalous dimension and \vec{Q} is the ordering wave vector for the three sublattice structure. Throughout the entire range $0 \leq r < 1.0$, we again find that scaling is satisfied for system sizes $L \leq 42$. Table I summarizes our results for the critical exponents in the range $0 \leq r \leq 1.0$. The critical exponents for which finite size scaling holds change with r

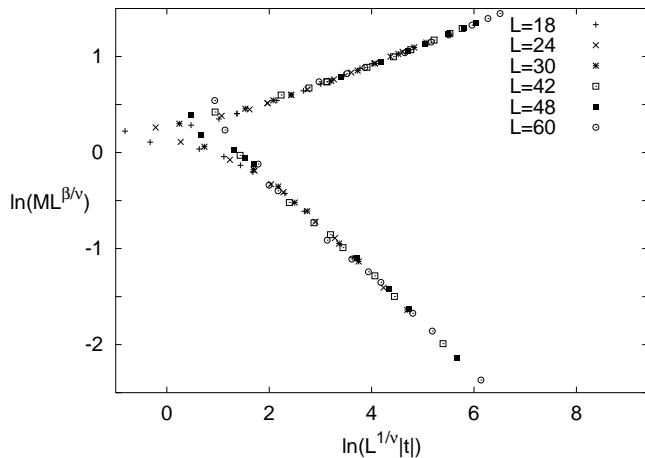


FIG. 1: Log-log finite size scaling plot of order parameter M for the $r = 1.0$ system. The transition temperature is $T^* = 1.7369$ and the exponent $\beta = 0.2134$. The best collapse of data was obtained for $\nu = 0.4817$.

showing clearly that universality is violated. Moreover η is always found to be negative — sometimes significantly, e.g. for $r = 0.2$ — which is impossible if the transition is of second order [1]. These results strongly suggest that scaling aborts ultimately — that is, very close to T^* — for all $r \in [0, 1]$ and that, therefore, the transitions are *all* of first order.

$r \geq 1.0$: the strong first order region. We now consider the region $r \geq 1.0$. As expected, the first order behavior found for the STAR, that is for $r \rightarrow \infty$, persists for finite r . We have been able to follow it down to $r \simeq 1.0$ by studying the probability distribution for the energy $P(E)$. This probability distribution is a useful quantity to locate first order transitions. Away from the transition point, one expects a Gaussian distribution in energy while at the transition point a double peak in $P(E)$ occurs if it is first order. This point can be located by finding the temperature where the weights under the peaks in $P(E)$ become equal. However distinguishing between a weak first order and a second order transition is rather delicate especially in case of a possible tricritical point. In order to make sure what type of phase transition the double peak structure represents, it is necessary to study the size dependence of the probability distribution $P(E)$. In the case of a first order transition, the separation of the peak energies E_1 and E_2 equals the latent heat up to $1/L$ corrections [17]. Thus two peaks remain separated with increased size L and, as shown in [18], become sharper.

We have found a double peaked structure in $P(E)$ for rigidity parameters $r = 1.0, 1.5, 2.0, 4.0, 6.0$ and 8.0 for linear sizes $L \leq 60$. As the value of r decreases, the size of the system where the double peak structure starts to appear increases. However, the energy autocorrelation time is less than 2000 MCS in this range. The dou-

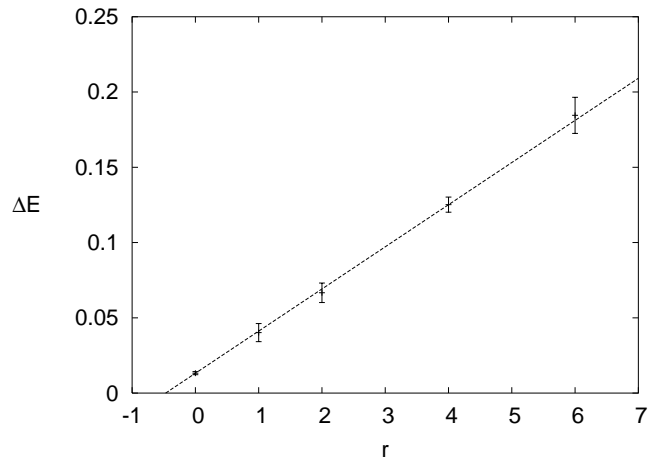


FIG. 2: The dashed line corresponds to a linear fit of the energy difference of peak maxima for $r = 1, 2, 4$ and 6 . The point at $r = 0$ was estimated from the histograms in figure 3.

ble peaked structure in $P(E)$, and thus the first order behavior, is apparent but only for lattice sizes $L > 48$ for $r = 1.0$. If we extrapolate to the thermodynamic limit, we can estimate the latent heat $\Delta E = |E_1 - E_2|$ at the transition. Using the values of ΔE for $r \geq 1.0$ and extrapolating to the more interesting small r region predicts that ΔE remains nonzero at $r = 0$ with an estimated value of 0.010 ± 0.002 . This behavior suggests that the phase transition at $r = 0$ might be weakly first order.

In figure 2 we plot ΔE vs r where it can be seen that it extrapolates linearly to the physically interesting limit of small r . The maximum size used for $r = 6$ was $L = 36$ and hence the errorbars are larger than those at smaller r . The value at $r = 0$ is finite indicating a weak first order transition. The extrapolation also predicts that ΔE vanishes at $r_0 = -0.47 \pm 0.02$. Our error bars for r_0 are compatible with $r = -0.5$, corresponding to the stacked Kagome lattice, for which one expects a completely different physics. We conclude that STA undergoes a very weak first order phase transition and that there is no tricritical point for all systems described by $H(r)$ with $r > -0.5$.

STA $r = 0$. In order to confirm our result of a non-zero latent heat at $r = 0$, we have studied the energy probability distribution for the $r = 0$ case using much larger system sizes. Figure 3 shows $P(E)$ at T^* for sizes $L = 87, 111$ and 138 . A double peak structure characteristic of a first order phase transition is now evident at these sizes. As the size of the system is increased, the peaks sharpen and the depth of the minimum between the peaks also increases. For these larger sizes the energy autocorrelation time increases significantly to values greater than 12000 MCS. This critical slowing down could perhaps be improved using overrelaxation or multi-

canonical histogram methods.[18] However, we estimate a value $\Delta E \sim 0.013 \pm 0.001$ from figure 3 which is in excellent agreement with the previous estimate 0.010 ± 0.002 obtained from the extrapolation of $\Delta E(r)$ from larger $r \geq 1.0$ to $r = 0$.

In conclusion, we have studied a system interpolating continuously between the XY STA and STAR models and find unambiguous evidence that the phase transitions in these systems is either of first order or weakly first order accompanied by scaling with exponents varying with r . These results provide strong arguments in favor of the nonperturbative approach to the physics of frustrated magnets [1] and suggest that, even if a fixed point exists, its relevance for STA-like compounds whose microscopic Hamiltonians are supposed to be well described by Eq. (1), is doubtful. Indeed, while the two — perturbative and nonperturbative — approaches both predict scaling in a transient regime near T^* , they differ in several ways. First, asymptotically, *i.e.* at T^* — the scaling behavior aborts in the nonperturbative scenario while it persists in the perturbative one since it is associated with a true continuous phase transition. Second, the weak first order transitions are generic in the nonperturbative scenario whereas they should be exceptional in the perturbative one [1]. Indeed, in the presence of a fixed point, systems undergoing weak first order phase transitions correspond, in the space of coupling constants, to initial conditions of the RG flow that are outside the basin of attraction of the fixed point but that lie in the vicinity of the separatrix between the first and second order regions. This behavior should not be generic since it implies a fine-tuning of the parameters of the microscopic Hamiltonian. Note however that one cannot completely exclude that, by varying another microscopic parameter like the ratio between the interlayer and intralayer coupling constants, the system be driven into the basin of

attraction of a fixed point.

The present work as well as the one performed by Itakura [11] predict a first order phase transition for STA. Previous numerical simulations failed to reach the asymptotic regime where the correlation length saturates, that is, where the scaling aborts. This suggests that the same phenomenon could occur in experiments, this time due to the difficulty to probe the close vicinity of T^* , and that all real materials also display weak first order transitions. This hypothesis is reinforced by the fact that the exponents found in our study are close to the experimental ones for STA compounds (see [1] and references therein). Let us consider for instance the exponent β which is the best measured one. Here we find a variation of β in the range $[0.213, 0.253]$ while for XY STA compounds one has, for instance, $\beta \simeq 0.228$ for CsMnBr_3 , $\beta \simeq 0.243$ for CsNiCl_3 and $\beta \simeq 0.23 - 0.25$ for CsCuCl_3 which has been finally found to undergo a first order transition when the study of the close vicinity of T^* has been refined.

An important open question concerns the Heisenberg case where there exists the same conflict between the perturbative and nonperturbative scenarios. However, according to the NPRG scenario, the transition should be even more weakly of first order for Heisenberg than for XY spins so that the controversy will be more difficult to settle.

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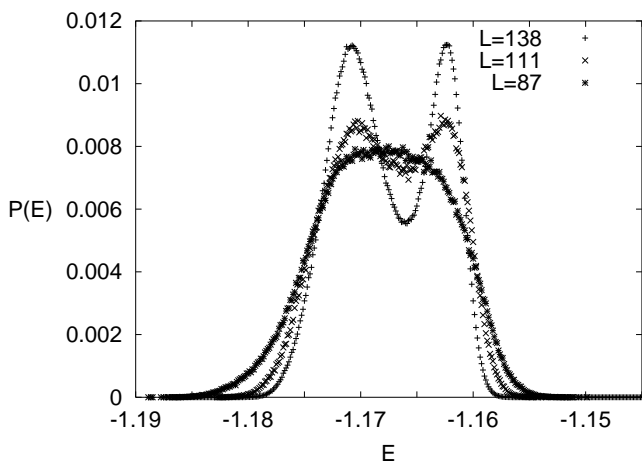


FIG. 3: $P(E)$ for STA XY model ($r = 0$) for $L = 87, 111$ and $L = 138$ at T^* .

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